CTT
Centre for
Trustworthy
Technology

A New Frontier for Drug Discovery and Development:

Artificial Intelligence and Quantum Technology

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About the Centre

The Centre for Trustworthy Technology is a part of the World Economic Forum's C4IR Network.

Our vision

Our vision is to empower all through the responsible integration and use of innovative and potentially disruptive technologies.

Our mission

Our mission is to guide organizations in understanding, preparing for, and leveraging transformative and trustworthy technologies, thereby promoting a future where technological innovation benefit all.

Our core values

Our core values include Collaboration, Global inclusivity, Human-Centered outcomes, Being Action-Oriented, Passionate and Committed to Learning & Educating.

Introduction

The pharmaceutical industry has always been on the cutting edge of adopting new technologies to enhance its drug discovery and development productivity.[i] The interface with Artificial Intelligence (AI) is transforming the entire process through target validation, compound screening, lead optimization and possibly even clinical trials. AI's ability to process vast amounts of data, build predictive models, and automate complex processes has allowed pharmaceutical companies to accelerate drug discovery, personalize treatments, and optimize manufacturing processes.[ii]

The transformational impact of AI in drug discovery is rapidly unfolding, with numerous companies from industry pioneers like Exscientia to innovative firms like Insilico Medicine, Evotec, and Schrödinger embracing this powerful technology.[iii] Since the landmark entry of the first AI-designed drug candidate in early 2020, the field witnessed over 100 AI-inclusive submissions to US Food and Drug Administration in 2021 alone.[iv] Insilico Medicine's use of generative AI to create a novel drug candidate to treat idiopathic pulmonary fibrosis entering Phase II trials is a notable success.[v] Equally remarkable is Absci Corporation creating and validating de*novo antibodies in silico* (via a computer).[vi] Recursion, a biotechnology company, announced in August of this year that in less than 90 days it has been able to predict protein interactions of 36 billion chemical compounds potentially accelerating the pace of drug discovery.[vii]

Recent drug design and development trends among leading traditional pharmaceutical companies unequivocally demonstrate collaboration, co-design, and innovation evolved into indispensable principles integral to shaping the industry's future landscape.[viii] These key principles are now at the forefront, steering success and propelling sustained growth within the realm of drug discovery and development. These are the initial sparks of a transformative revolution now igniting, signaling the onset of significant change.

A recent report highlighted even modest enhancements in early-stage drug development success rates facilitated by artificial intelligence and machine learning could culminate in approximately 50 novel therapies within a decade. This signifies a market opportunity exceeding $50 billion.[ix] Notably, however, a significant impediment to fully integrating AI and unlocking its potential in drug discovery is the prevailing lack of trust within the industry.[x]

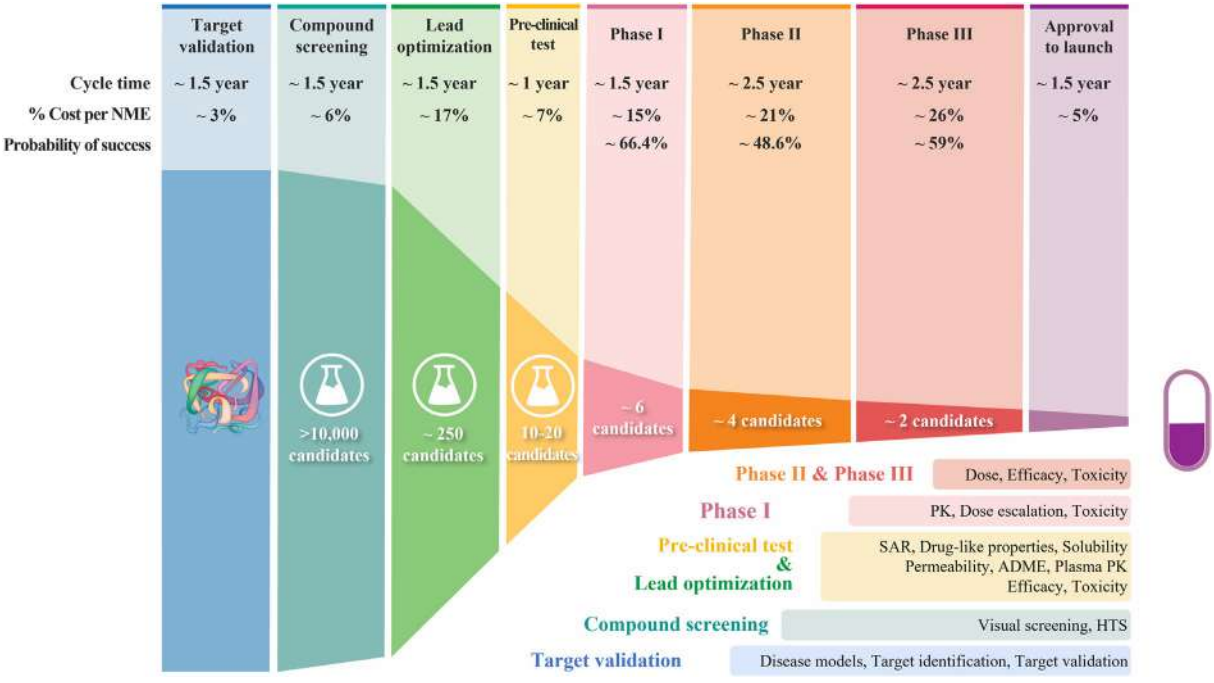
Future advances in Quantum computing are poised to provide another revolutionary shift in the industry. Quantum technology has the potential to unravel complex biological phenomena which are currently unseen by classical computers. For instance, in July 2023 Gero, a biotech company with expertise in aging and longevity, highlighted quantum computing's potential to enhance drug design and discovery efficiency.[xi] Its research led to the harnessing of 2331 novel chemical structures.[xii] The quantum leap could further elevate the productivity in areas such as molecular modeling and optimization, opening new frontiers in pharmaceutical innovation.[xiii]

This thrilling frontier comes with profound responsibilities. At stake are human lives, and the risks are substantial. As we stand on the cusp of an era where medical miracles seem within reach, ensuring the trustworthiness and ethical application of these emerging technologies must be the unwavering priority for every stakeholder in the field. The promise is immense, but so must be our diligence and care.

Demystifying Drug Development

Drug discovery and development is a complex, costly, and time-consuming process. The average cost of bringing a drug to market has varied estimates, yet even conservative estimates put the figure at over one billion dollars.[xiv] The average timeline for this process stands at a decade with a success rate of approximately 10%.[xv] The substantial financial investments, elongated time frame, and high failure rates are intrinsic challenges to this process. To fathom how AI and quantum computing can potentially revolutionize drug discovery, it is essential to understand this labyrinthine process.

The complex process of drug development commences with target identification and validation to find the right biological target, such as a protein that plays a key role in the disease process. This is followed by screening for lead discovery which involves testing thousands of potential compounds to see their effect on the biological target. Then comes optimization, where identified leads may be chemically modified to enhance their properties, such as binding affinity, selectivity, solubility, and stability. Optimization is followed by preclinical testing and several stages of clinical trials expanded upon below. Each step demands meticulous analysis, careful experimentation, and rigorous evaluation to ensure the safety and efficacy of the potential therapeutic compound.



xvi

Pre-Discovery Stage

During this phase, research scientists engage in fundamental studies to identify a specific macromolecule—often a protein—involved in the pathophysiology of the disease of interest. This macromolecule, usually termed a 'therapeutic target', signifies the initial link between biological mechanisms and pathological states.

Drug Discovery

This phase involves the identification and testing of therapeutic agents capable of modifying the function of the target. This includes using computers to model drug-target interactions, doing tests in labs, studying tissues or organs, and testing on rodents. Both pre-discovery and drug discovery stages usually take 3-5 years of research.

Preclinical Phase

During this phase, potential drugs undergo rigorous testing to ascertain their safety profiles and determine their candidacy for further trials. The preclinical stage takes 1-3 years where best potential drug candidates are chosen through more computer modelling, lab tests, and animal testing. Once the safety checks are done, an application called an *'Investigational New Drug' (IND) application* is submitted to health authorities like the Food and Drug Administration in the U.S.A. This application includes information about safety of drug, its composition, manufacturing process, the plan for clinical trials etc.

Clinical Trial Phase

In this stage, studies which engage with human subjects begin with an objective to determine both the safety and efficacy of potential drug candidates. There are typically four stages of these trials. A drug must succeed in showing its efficacy and safety at each stage. Three of these stages occur at this point, and a final one after the approval of the drug by regulators, explained below. Each stage progressively enrolls more individuals to test the drug for various parameters of safety and efficacy. Iteratively, each stage also has higher thresholds of information disclosure about the drug to those in the trial and parameters for clearing the stage. This stage usually lasts 4-7 years. After the completion of Phase 3 trials, a '*New Drug Application' (NDA)* is submitted to concerned health authorities to demonstrate safety and efficacy of the potential drug candidate.

Review

Concerned health authorities diligently review the trial data and take a decision regarding market approval. A positive review results in the release of the drug to the market and its subsequent administration to patients.

Pharmacovigilance

The final step in the process is commonly referred to as pharmacovigilance or 'Phase 4' of the clinical trial. Even after market approval, the approved drugs undergo continued surveillance to monitor for any potential side effects or adverse reactions that may manifest over time resulting from the treatment. This ensures the long-term safety and efficacy of the new treatment in a broader patient population.

Unleashing Potential:

AI and Quantum Technologies Shaping the Future of Drug Discovery

The traditionally lengthy process of drug discovery and development is undergoing a transformation with the integration of AI and the application of quantum technology in the absence of fault tolerant quantum computers. Specific advances within these cutting-edge fields are making it possible to intervene in various stages of the process and reshaping the entire landscape of pharmaceutical research. Together, they promise to streamline the drug discovery and development process, providing targeted solutions that boost efficiency and optimization from initial research to clinical trials.

AI's Reach in Drug Discovery & Development

AI has contributed to a pole vault in efficiency and efficacy involved in drug discovery and development with varied ancillary developments in the last few years. First, deep learning enabled comprehensive analysis of massive chunks of data to find coherent patterns and fruitful inferences.[xvii] Secondly, there has been a Cambrian explosion of data relevant to the life sciences including genomic[xviii] (genes related), proteomic[xix] (proteins related) and transcriptomic[xx] (RNA related) data ready to be utilized to innovate anew.[xxi] Thirdly, the computational prowess of Graphics Processing Units (GPUs) catalyzed a shift by augmenting the rapid analysis and processing of vast datasets integral to biomedical research.[xxii] Finally, a revolutionary innovation emerged with Generative AI, which has the potential to simulate and predict molecular structures and interactions aiding drug design.[xxiii]

These developments synergistically contribute to the pharmaceutical research revolution through accelerated timelines, reduced costs, and enhanced precision.

Deep Learning

is a subset of machine learning that mimics the workings of the human brain in processing data, recognizing patterns, and making decisions. Deep Learning makes use of 'neural networks' which consist of many layers to analyze various facets of data. Deep Learning models can analyze vast chemical spaces and biological data to predict how different compounds can interact with targets in the body. In developing new drugs, Deep Learning can simulate how drugs will interact with their targets, help optimize drug formulations, and predict potential side effects.

Big Data

The proliferation of genomic, transcriptomic, proteomic, and other data sets, sourced both from healthy individuals and those afflicted with specific diseases, represents a substantial opportunity to guide the selection of biological targets. The complexity and diversity of origins in these data sets make them particularly amenable to analysis using AI/ML approaches, unlocking potential new insights and understanding in the field.

Graphics Processing Units (GPUs)

are specific hardware designed and built to process calculations necessary for rendering images, animations, and video. Unlike Central Processing Units (CPUs) that manage general-purpose tasks, GPUs are optimized for parallel processing, which means they can execute many calculations simultaneously.

Generative AI

functions to create new data instances basis training on a substantive dataset. It has emerged as a powerful tool in drug discovery and development. It works by training on existing chemical structures and biological data, following which it has the ability to 'generate' new molecular structures that could potentially be effective as therapeutic agents. Through this process, generative AI can rapidly explore vast chemical spaces, identifying novel compounds that might take human researchers much longer to discover. It enables the optimization of existing drug candidates by suggesting modifications to enhance binding affinity, reduce toxicity, or improve other pharmacological properties.

Key Advantages of AI:

Initial Discovery Phases

- **Process rationalization and project management:** AI is being deployed to streamline operations and facilitate intricate project management through the drug discovery and development phases.

- **Information consolidation:** AI aids to assimilate and collate vast data sets, providing researchers with concise summaries and key insights, thereby simplifying the interpretation of complex biomedical data for researchers.

- **Deciphering complex biological systems aiding target discovery:** By utilizing methods such as systems biology and chemogenomic, AI is elucidating intricate biological systems, thus enhancing our comprehension of these complex 'languages' of biology. As a result, AI facilitates a clearer understanding of targets and potential pathways for modulation, thereby contributing significantly to the refinement of the target product profile.

- **Molecular simulations:** AI is being leveraged to minimize the necessity for hands-on testing of potential drug compounds. It helps predict the interactions between Active Pharmaceutical Ingredients (APIs) and target receptors by calculating the binding affinity between an API and its target.[xxiv] Through high-precision molecular simulations, tests can be conducted entirely using computer systems (i.e., in silico).[xxv] This helps situate each compound relative to the desired final drug specifications within a complex multidimensional landscape.[xxvi] This approach avoids the substantial expenses associated with conventional chemical methodologies.

- **De Novo drug design:** AI is revolutionizing the way new chemical structures are proposed by automating the creation of novel compounds that best align with a targeted molecular profile.[xxvii]

- **Tailoring for key properties:** AI is being used to propose potential therapeutic agents while adhering to various constraints of ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) parameters.[xxviii]

- **Candidate Drug Prioritization:** After identifying a collection of promising "lead" drug compounds, AI comes into play to evaluate and organize these molecules, ranking them in order of priority for subsequent analysis.[xxix]

Drug Development Phases

- **Modelling for efficacy:** By synergizing AI with data mining techniques, AI can help model drug-target interactions.[xxx] This aids in expeditiously exploring potential efficacy of drugs basis pharmacokinetics (what the body does to the drug including the absorption, distribution, metabolism, and excretion of the drug) and pharmacodynamics (what the drug does to the body essentially helping to us to understand how the drug exerts its therapeutic effects and any adverse effects that may occur)[xxxi]

- **Adverse effect explanation:** AI can help forecast potential adverse events[xxxii] associated with a compound basis its specificity and affinity for a particular target. This allows for a nuanced understanding of how the compound may interact with the target to help anticipate possible unwanted side effects.

- **Patient diversity and precision medicine:** AI plays a role in unraveling the reasons behind different responses to the same medication across diverse individuals. This understanding is contributing to the advancement of personalized medicine.[xxxiii]

- **Efficient Clinical Trials:** AI can be used to sift through massive amounts of data from hands-on tests (like clinical trials) and hands-off studies (like observational research) to determine how safe and effective a drug is. It can help shape new types of tests, like remote clinical trials, and make sense of real-world data from sources like medical records. It can also help understand data from digital health tools such as wearables used in studies. It can assist in identifying optimal patient populations for inclusion in clinical trials, thereby enhancing the relevance and informativeness of the results obtained. Ultimately, AI can make the process of running clinical trials smoother and more efficient.[xxxiv]

- **Digital Twins:** This concept leverages AI to create a digital avatar of a biological system or an individual to run simulations of drugs efficacy upon. This approach could facilitate predictions regarding disease progression, efficacy of current treatments, or individual responses to new therapeutic agents.[xxxv] While this concept holds significant promise, it is currently confronted with numerous challenges and is a hotbed for ongoing research.

Quantum on the Anvil

Traditional computing methods struggle to precisely describe quantum systems for the pharmaceutical sector.[xxxvi] Even so, classical machine learning yielded success in drug discovery. However, its computational demands are substantial. Recently, researchers are exploring quantum computing in relation to ML, leading to the emergence of quantum machine learning (QML).[xxxvii] QML combines the principles of quantum computing with traditional machine learning algorithms, enabling enhanced computational efficiency, and the potential to solve complex problems currently intractable for classical computers.[xxxviii] Such advances lead to brimming potential for drug discovery and development.

Deciphering the immune system down to its intricate details becomes a possibility with quantum technology. Molecules (potential drugs) operate on principles found in quantum physics.[xxxix] Quantum technology has the potential to augment the predictive and simulating ability to comprehensively understand both the target's and drug candidate's precise models and interactions.[xl] Hence, quantum technology can boost efficacy and efficiency across the of drug discovery and development chain.[xli]

Quantum technology leverages the principles of quantum mechanics, which governs the behavior of matter and energy on the smallest scales. Unlike classical computing, where information is processed in binary bits (0 or 1), quantum technology uses quantum bits, or qubits, that can exist in multiple states simultaneously. This property, known as superposition, facilitates processing a high number of possibilities simultaneously. Thereby making quantum computations exponentially faster for specific tasks.

Quantum entanglement, another core principle, enables qubits to be interconnected so that the state of one instantaneously influences the state of another, no matter the distance between them. This facilitates a high level of coordination between qubits and helps in parallel computation. Together these principles in quantum technology allow for a major boost in the processing power available to us.

While still in early stages, the availability and accessibility to quantum technologies will bring about productivity boost in this process.

Key Advantages of Quantum Technology:

- **Machine Learning and Predictive Modeling:** Quantum-enhanced machine learning will aid in analyzing large datasets. It will augment our ability to correctly model potential drug candidate properties, target modulation techniques, and drug-target interactions.
- **Enhanced Accuracy in Prediction:** Quantum technologies can lead to higher accuracy in modeling human immunology and predicting viable drug candidates.
- **Rapid Prediction of Drug Properties:** It will allow for faster predictions of toxicity and efficacy of potential drug candidates.
- **Efficient Optimization of Drug Candidates:** It will efficiently handle complex optimization problems which are key challenges in drug discovery and development. It will help in identifying promising candidates, reducing failure rates.
- **Cost-Effective Testing Processes:** It can lead to new innovative, economical, and efficient testing of potential drug candidates.

Trustworthy 'VITAL PIECES'

The The integration of AI and the emergence of quantum technologies set the stage for transformative changes in drug discovery. These technologies promise to be game changers, substantially boosting the speed and efficiency of drug discovery and development. The urgency for faster access to essential medications cannot be overstated. However, ensuring this integration is done in a trustworthy manner is paramount.

The drug discovery and development timeline serves as a practical framework but also as a safeguard, embedding the highest level of trust in consumer-facing pharmaceutical products. The time taken in the entire process can itself be considered an integral mechanism for building trust. Consequently, the acceleration promised by AI and quantum technologies raises critical questions about maintaining trust in the face of newfound speed and efficiency.

Within this context, several **'VITAL PIECES'** in this domain must be ensured by Pharmaceutical Companies:

- **Verifying Application:** Although technology's integration into early drug development is swift, its use during human-centric phases, like clinical trials, must be handled with caution. Ensuring zero compromise between productivity and the possibility of adverse human impact is paramount.
- **Integrated Risk Planning:** A comprehensive risk mitigation plan must be tailor-made for AI and Quantum use in pharmaceutical companies, emphasizing documentation, transparency, and clear justifications for procedural deviations.
- **Trusted Models:** Continuously assessing AI models with audits and human oversight should be considered essential to guarantee their reliability, relevance, and consistency over time.
- **Avoiding Bias:** Vigilance in data handling is paramount to prevent biases, ensuring data quality, representativeness, and relevance for the drug discovery and development process. It is important to develop a robust data strategy for the process's integrity and relevance.
- **Leveraging Transparency:** Chartering a clear communication policy on developments with regulators should be taken as a key responsibility to demonstrate the utility and risks of new technologies.
- **Partnered Design:** Co-designing solutions using a multidisciplinary lens, involving life science professionals, ethicists, and tech experts amongst others, should be pursued to foster robustness in the AI and Quantum integration process.
- **Inherent Principles:** Emphasizing adherence to guiding principles throughout the drug discovery cycle, with safety as a top priority, is crucial. We have seen these being pursued by industry bodies[xlii] and certain companies[xliii] [xliv]. A broad industry-wide adoption of a principles-based approach must be considered.
- **Ethical Cooperation:** During AI and Quantum's early integration, sharing best practices and safety mechanisms would be pivotal for responsible and trustworthy adoption.
- **Collaborative Ecosystem**: Establishing an environment which encourages partnership to enable optimal and responsible integration of AI and Quantum and embedding checks and balances.
- **Ensure Adherence:** Committing to educating the entire workforce to enact the ethical principles, risk mitigation strategies and data strategy should be prioritized.
- **Shared Vision:** Recognizing the immense benefits and potential risks and moving ahead with a shared vision to ensure faster access to drugs but not at the cost of trustworthiness of the entire system will be crucially important.

V Verifying Application — Exercise caution and vigilance during human-centric evaluations i.e., clinical trials.

I Integrated Risk Planning — Implement a risk mitigation plan.

T Trusted Models — Continuous audit and oversight

A Avoiding Bias — Promote safeguards against bias

L Leveraging Transparency — Undertake transparent communication with regulators

P Partnered Design — Encourage multi-disciplinary collaboration

I Inherent Principles — Adhere to guiding principles

E Ethical Cooperation — Share safety mechanisms and best practices

C Collaborative Ecosystem — Foster a collaborative environment

E Ensure Adherence — Educate the workforce to action principles

S Shared Vision — Share risks and benefits

Conclusion

The potential benefits of integrating AI and quantum technologies into the pharmaceutical industry are vast. However, this transition must be navigated with caution, ethical rigor, and a holistic consideration of the unique challenges and responsibilities intrinsic to drug discovery and development. Ensuring the integration of these technologies aligns with established principles and ethical considerations will be key to realizing the transformative potential without compromising the trust and safety foundational to the industry.

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